

Two-electron self-energy contribution to the ground state energy of heliumlike ions

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Abstract

The two-electron self-energy contribution to the ground state energy of heliumlike ions is calculated both for a point nucleus and an extended nucleus in a wide interval of Z . All the two-electron contributions are compiled to obtain most accurate values for the two-electron part of the ground state energy of heliumlike ions in the range $Z = 20 - 100$. The theoretical value of the ground state energy of $^{238}\text{U}^{90+}$, based on currently available theory, is evaluated to be $-261382.9(8)$ eV, without higher order one-electron QED corrections.

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1 Introduction

The recent progress in heavy-ion spectroscopy provides good perspectives for testing the quantum electrodynamics in a region of strong electric field. In [1, 2] the two-electron contribution to the ground-state energy of some heliumlike ions was measured directly by comparing the ionization energies of heliumlike and hydrogenlike ions. In such an experiment the dominating one-electron contributions are completely eliminated. Though the accuracy of the experimental results is not high enough at present, it is expected [2] that the experimental accuracy will be improved by up to an order of magnitude in the near future. This will provide testing the QED effects in the second order in α .

In this paper we calculate the ground state two-electron self-energy correction in the second order in α in the range $Z = 20 - 100$. Calculations of this correction were previously performed for some ions for the case of a point nucleus by Yerokhin and Shabaev [3] and for an extended nucleus by Persson *et al.* [4, 5]. Contrary our previous calculation of this correction, the full-covariant scheme, based on an expansion of the Dirac-Coulomb propagator in terms of interactions with the external potential [6, 7], is used in the present work. This technique was already applied by the authors to calculate the self-energy correction to the hyperfine splitting in hydrogenlike and lithiumlike ions [8, 9].

The paper is organized as follows. In the Sec. 2 we give a brief outline of the calculation of the two-electron self-energy contribution. In the Sec. 3 we summarize all the two-electron contributions to the ground state energy of heliumlike ions. The relativistic units ($\hbar = c = 1$) are used in the paper.

2 Self-energy contribution

The two-electron self-energy contribution is represented by the Feynman diagrams in Fig.1. The formal expressions for these diagrams can easily be derived by the two-time Green function method [10]. Such a derivation was discussed in detail in [3]. The diagrams in Fig.1a are conveniently divided into irreducible and reducible parts. The reducible part is the one in which the intermediate state energy (between the self-energy loop and the electron-electron interaction line) coincides with the initial state energy. The irreducible part is the remaining one. The contribution of the irreducible part can be written in the same form as the first order self-energy

$$\Delta E_{\text{irred}} = 2 \left[\langle \xi | \Sigma_R(\varepsilon_a) | a \rangle + \langle a | \Sigma_R(\varepsilon_a) | \xi \rangle \right], \quad (1)$$

where $\Sigma_R(\varepsilon)$ is the regularized self-energy operator, ε_a is the energy of the initial state a , and $|\xi\rangle$ is a perturbed wave function defined by

$$|\xi\rangle = \sum_{\varepsilon_n \neq \varepsilon_a} \frac{|n\rangle [\langle nb | I(0) | ab \rangle - \langle nb | I(0) | ba \rangle]}{\varepsilon_a - \varepsilon_n}. \quad (2)$$

Here $I(\omega)$ is the operator of the electron-electron interaction. The calculation of the irreducible part is carried out using the scheme suggested by Snyderman [6] for the first order self-energy contribution.

The reducible part is grouped with the vertex part (Fig.1b). For the sum of these terms the following formal expression is obtained

$$\begin{aligned} \Delta E_{\text{vr}} = & 2\alpha^2 \sum_P (-1)^P \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \int d\mathbf{x} d\mathbf{y} d\mathbf{z} \frac{e^{i|\omega||\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|} \\ & \times \left[\psi_{Pa}^\dagger(\mathbf{x}) \alpha_\nu \int d\mathbf{z}_1 \psi_{Pb}^\dagger(\mathbf{z}_1) \frac{\alpha_\mu}{|\mathbf{z}-\mathbf{z}_1|} \psi_b(\mathbf{z}_1) \right. \\ & \times G(\varepsilon_a - \omega, \mathbf{x}, \mathbf{z}) \alpha^\mu G(\varepsilon_a - \omega, \mathbf{z}, \mathbf{y}) \alpha^\nu \psi_a(\mathbf{y}) \\ & - \langle PaPb | \frac{1 - \boldsymbol{\alpha}_1 \boldsymbol{\alpha}_2}{r_{12}} | ab \rangle \\ & \left. \times \psi_a^\dagger(\mathbf{x}) \alpha_\nu G(\varepsilon_a - \omega, \mathbf{x}, \mathbf{z}) G(\varepsilon_a - \omega, \mathbf{z}, \mathbf{y}) \alpha^\nu \psi_a(\mathbf{y}) \right]. \quad (3) \end{aligned}$$

Here the first term corresponds to the vertex part, and the second one corresponds to the reducible part. $G(\varepsilon, \mathbf{x}, \mathbf{z})$ is the Coulomb Green function, α is the fine structure constant, $\alpha^\mu = (1, \boldsymbol{\alpha})$, $\boldsymbol{\alpha}$ are the Dirac matrices, a and b are the $1s$ states with spin projection $m = \pm \frac{1}{2}$, and P is the permutation operator.

According to the Ward identity the counterterms for the vertex and reducible parts cancel each other, and, so, the sum of these terms regularized in the same covariant way is ultraviolet finite. To cancel the ultraviolet divergences analytically we divide ΔE_{vr} into two parts $\Delta E_{\text{vr}} = \Delta E_{\text{vr}}^{(0)} + \Delta E_{\text{vr}}^{\text{many}}$. The first term is $\Delta E_{\text{vr}}^{(0)}$ with both the bound electron propagators replaced by the free propagators. It does not contain the Coulomb Green functions and can be evaluated in the momentum representation, where all the ultraviolet divergences are explicitly cancelled using a standard covariant regularization procedure. The remainder $\Delta E_{\text{vr}}^{\text{many}}$ does not contain ultraviolet divergent terms and is

calculated in the coordinate space. The infrared divergent terms are handled introducing a small photon mass μ . After these terms are separated and cancelled analytically the limit $\mu \rightarrow 0$ is taken.

In practice the calculation of the self-energy contribution is made using the shell model of the nuclear charge distribution. Since the finite nuclear size effect is small enough even for high Z (it constitutes about 1.5 percent for uranium), an error due to incompleteness of such a model is negligible. The Green function for the case of the shell nucleus in the form presented in [11] is used in the calculation. To calculate the part of ΔE_{irred} with two and more external potentials, we subtract from the Coulomb-Dirac Green function the first two terms of its potential expansion numerically. To obtain the second term of the expansion it is necessary to evaluate a derivative of the Coulomb Green function with respect to Z at the point $Z = 0$. We handle it using some algorithms suggested in [12].

The numerical evaluation of $\Delta E_{\text{vr}}^{\text{many}}$ is the most time consuming part of the calculation. The energy integration is carried out using the Gaussian quadratures after rotating the integration contour into imaginary axis. To achieve a desirable precision it is sufficient to calculate 12-15 terms of the partial wave expansion. The remainder is evaluated by fitting the partial wave contributions to a polynomial in $\frac{1}{l}$. A contribution arising from the intermediate electron states which are of the same energy as the initial state is calculated separately using the B-spline method for the Dirac equation [13]. The same method is used for the numerical evaluation of the perturbed wave function $|\xi\rangle$ in equation (1).

Table 1 gives the numerical results for the two-electron self-energy contribution to the ground state energy of heliumlike ions expressed in terms of the function $F(\alpha Z)$ defined by

$$\Delta E = \alpha^2 (\alpha Z)^3 F(\alpha Z) mc^2 \quad (4)$$

To the lowest order in αZ , $F = 1.346 \ln Z - 5.251$ (see [3] and references therein). The results for a point nucleus and an extended nucleus are listed in the third and fourth columns of the table, respectively. In the second column the values of the root-mean-square (rms) nuclear charge radii used in the calculation are given [14, 15]. In the fifth column the results for an extended nucleus expressed in eV are given to be compared with the ones of Persson *et al.* [4] listed in the last column of the table. A comparison of the present results for a point nucleus with the ones from [3] finds some discrepancy for the contribution which corresponds to the Breit part of the electron-electron interaction. This discrepancy results from a small spurious term arising in the non-covariant regularization procedure used in [3].

3 The two-electron part of the ground state energy

In the Table 2 we summarize all the two-electron contributions to the ground state energy of heliumlike ions. In the second column of the table the energy contribution due to one-photon exchange is given. Its calculation is carried out for the Fermi model of the nuclear charge distribution

$$\rho(r) = \frac{N}{1 + \exp((r - c)/a)} \quad (5)$$

with the rms charge radii listed in the Table 1. Following to [14], the parameter a is chosen to be $a = \frac{2.3}{4\ln 3}$ fm. The parameters c and N , with a good precision, are given by (see, e.g., [16])

$$c = \frac{1}{\sqrt{3}} \left[\left(4\pi^4 a^4 - 10\langle r^2 \rangle \pi^2 a^2 + \frac{25}{4} \langle r^2 \rangle^2 \right)^{\frac{1}{2}} - 5\pi^2 a^2 + \frac{5}{2} \langle r^2 \rangle \right]^{\frac{1}{2}}, \quad (6)$$

$$N = \frac{3}{4\pi c^3} \left(1 + \frac{\pi^2 a^2}{c^2} \right)^{-1}. \quad (7)$$

Except for $Z=83, 92$, the uncertainty of this correction is obtained by a one percent variation of the rms radii. In the case $Z=92$ ($\langle r^2 \rangle^{1/2} = 5.860(2)$ fm [17]), the uncertainty of this correction is estimated by taking the difference between the corrections obtained with the Fermi model and the homogeneously charged sphere model of the same rms radius. For $Z = 83$, the uncertainty comes from both a variation of the rms radius by 0.020 fm (it corresponds to a discrepancy between the measured rms values [14]) and the difference between the Fermi model and the homogeneously charged sphere model.

The energy contribution due to two-photon exchange is divided into two parts. The first one ("non-QED contribution") includes the non-relativistic contribution and the lowest order ($\sim (\alpha Z)^2$) relativistic correction, which can be derived from the Breit equation. This is given by the first two terms in the αZ -expansion [18, 19, 20]

$$\Delta E_{\text{non-QED}} = \alpha^2 [-0.15766638 - 0.6356(\alpha Z)^2] mc^2 \quad (8)$$

and is presented in the third column of the Table 2. The second part which we refer to as the "QED contribution" is the residual and is given in the fourth column of the table. The data for the two-photon contribution for all Z , except for $Z = 92$, are taken from [21], interpolation is made when it is needed. For $Z = 92$ data from [22] are taken. In the fifth column of the table the results of the present calculation of the two-electron self-energy contribution are given. The two-electron vacuum polarization contribution taken from [23] is listed in the sixth column. In the seventh column the "non-QED part" of the energy correction due to exchange of three and more photons is given. This correction is evaluated by summing the Z^{-1} expansion terms for the ground state energy of heliumlike ions beginning from Z^{-3} . The coefficients of such an expansion are taken to zeroth order in αZ from [18] and to second order in αZ from [20]. The three and more photons QED correction has not yet been calculated. We assume that the uncertainty due to omitting this correction is of order of magnitude of the total second-order QED correction multiplied by factor Z^{-1} . It is given in the eighth column of the table. The two-electron nuclear recoil correction is estimated by reducing the one-photon exchange contribution by the factor $(1 - m/M)$. Such an estimate corresponds to the non-relativistic treatment of this effect and takes into account that the mass-polarization correction is negligible for the $(1s)^2$ state [20]. This correction and its uncertainty, which is taken to be 100% for high Z , are included into the total two-electron contribution. The two-electron nuclear polarization effect is expected to be negligible for the ground state of heliumlike ions. In the last column the total two-electron part of the ground state energy of heliumlike ions is given.

In the Table 3 our results are compared with the experimental data [1, 2] and the results of previous calculations based on the unified method [20], the all-order relativistic many body perturbation theory (RMBPT) [24], the multiconfiguration Dirac Fock treatment

[25], and RMBPT with the complete treatment of the two-electron QED correction [4, 5]. Data in the third column of the table are taken from [4] for $Z = 54, 92$ and from [5] for other Z . The one-electron contribution from [15] is subtracted from the total ionization energies presented in [24, 20] to obtain the two-electron part.

In the Table 4 we present the theoretical contributions to the ground state energy of $^{238}\text{U}^{90+}$, based on currently available theory. The uncertainty of the one-electron Dirac-Coulomb value comes from the uncertainty of the Rydberg constant (we use $hcR_\infty = 13.6056981(40)$ eV, $\alpha = 1/137.0359895(61)$). The one-electron nuclear size correction for the Fermi distribution with $\langle r^2 \rangle^{1/2} = 5.860$ fm gives 397.62(76) eV. The uncertainty of this correction is estimated by taking the difference between the corrections obtained with the Fermi model and the homogeneously charged sphere model of the same rms radius [26]. The nuclear recoil correction was calculated to all orders in αZ by Artemyev *et al.* [27]. The uncertainty of this correction is chosen to include a deviation from a point nucleus approximation used in [27]. The one-electron nuclear polarization effect was evaluated by Plunien and Soff [28] and by Nefiodov *et al.* [29]. The values of the first order self-energy and vacuum polarization corrections are taken from [30] and [31], respectively. The two-electron corrections are quoted from the Table 2. The higher order one-electron QED corrections are omitted in this summary since they have not yet been calculated completely. We expect they can contribute within several electron volts.

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Table 1: The two-electron self-energy contribution to the ground state energy of heliumlike ions. The function $F(\alpha Z)$ is defined by equation (4).

| Z | $\langle r^2 \rangle^{1/2} [\text{fm}]$ | F [point.nucl.] | F [ext.nucl.] | ΔE [eV] (this work) | ΔE [eV] (Ref. [4]) |
|-----|---|-------------------|-----------------|-----------------------------|----------------------------|
| 20 | | -1.7134(3) | | -0.1449 | |
| 30 | 3.928 | -1.3889(3) | -1.3887(3) | -0.3965(1) | |
| 32 | 4.072 | -1.3448(3) | -1.3446(3) | -0.4659(1) | -0.5 |
| 40 | 4.270 | -1.2115(3) | -1.2112(3) | -0.8197(2) | |
| 50 | 4.655 | -1.1140(3) | -1.1134(3) | -1.4717(4) | |
| 54 | 4.787 | -1.0907(3) | -1.0898(3) | -1.8146(5) | -1.8 |
| 60 | 4.914 | -1.0692(3) | -1.0679(3) | -2.4391(7) | |
| 66 | 5.224 | -1.0625(3) | -1.0603(3) | -3.223(1) | -3.2 |
| 70 | 5.317 | -1.0657(3) | -1.0629(3) | -3.855(1) | |
| 74 | 5.373 | -1.0752(3) | -1.0712(3) | -4.590(1) | -4.6 |
| 80 | 5.467 | -1.1014(3) | -1.0951(3) | -5.929(2) | |
| 83 | 5.533 | -1.1205(3) | -1.1124(3) | -6.726(2) | -6.7 |
| 90 | 5.645 | -1.1830(3) | -1.1682(3) | -9.005(2) | |
| 92 | 5.860 | -1.2062(4) | -1.1878(4) | -9.780(3) | -9.7 |
| 100 | 5.886 | -1.3307(6) | -1.2929(6) | -13.671(6) | |

Table 2: Various components of the two-electron contribution to the ground-state energy of helium-like ions (in eV).

| Z | 1-ph. exch. | 2-ph. exch. non-QED | 2-ph. exch. QED | Self energy | Vac. pol. | ≥ 3 ph. non-QED | ≥ 3 ph. QED | Total contr. |
|-----|-------------|------------------------|--------------------|----------------|--------------|-------------------------|---------------------|--------------|
| 20 | 345.76 | -4.66 | 0.01 | -0.15 | 0.01 | 0.03 | ± 0.01 | 341.00(1) |
| 30 | 529.42 | -5.12 | 0.04 | -0.40 | 0.04 | 0.03 | ± 0.01 | 524.00(1) |
| 32 | 567.61 | -5.23 | 0.04 | -0.47 | 0.04 | 0.03 | ± 0.01 | 562.02(1) |
| 40 | 726.64 | -5.76 | 0.07 | -0.82 | 0.09 | 0.03 | ± 0.02 | 720.24(2) |
| 50 | 943.09 | -6.59 | 0.10 | -1.47 | 0.19 | 0.04 | ± 0.02 | 935.35(2) |
| 54 | 1036.56 | -6.98 | 0.10 | -1.82 | 0.26 | 0.04 | ± 0.03 | 1028.16(3) |
| 60 | 1185.73(1) | -7.61 | 0.09 | -2.44 | 0.38 | 0.04 | ± 0.03 | 1176.19(3) |
| 66 | 1347.45(1) | -8.30 | 0.06 | -3.22 | 0.56 | 0.05 | ± 0.04 | 1336.58(4) |
| 70 | 1463.43(1) | -8.80 | 0.02 | -3.86 | 0.71 | 0.05 | ± 0.05 | 1451.55(5) |
| 74 | 1586.93(2) | -9.33 | -0.04(1) | -4.59 | 0.91 | 0.05 | ± 0.05 | 1573.92(6) |
| 80 | 1788.43(3) | -10.19 | -0.19 | -5.93 | 1.30 | 0.06 | ± 0.06 | 1773.47(7) |
| 83 | 1897.56(1) | -10.64 | -0.30(1) | -6.73 | 1.55 | 0.06 | ± 0.07 | 1881.50(7) |
| 90 | 2178.25(7) | -11.75 | -0.65 | -9.01 | 2.34 | 0.06 | ± 0.08 | 2159.24(11) |
| 92 | 2265.88(1) | -12.09 | -0.79 | -9.78 | 2.63 | 0.06 | ± 0.09 | 2245.92(9) |
| 100 | 2659.8(2) | -13.50 | -1.58 | -13.67(1) | 4.25 | 0.07 | ± 0.11 | 2635.4(2) |

Table 3: Two-electron contribution to the ground state energy of some helium-like ions (in eV).

| Z | Present work | Persson <i>et.al</i> [4, 5] | Indelicato [25] | Plante <i>et al.</i> [24] ^a | Drake [20] | Experiment [1, 2] |
|-----|--------------|--------------------------------|--------------------|---|---------------|----------------------|
| 32 | 562.02(1) | 562.02(10) | 562.1 | 562.1 | 562.1 | 562.5(1.6) |
| 54 | 1028.16(3) | 1028.2 | 1028.2 | 1028.4 | 1028.8 | 1027.2(3.5) |
| 66 | 1336.58(4) | 1336.59(10) | 1336.5 | 1337.2 | 1338.2 | 1341.6(4.3) |
| 74 | 1573.92(6) | 1573.93(10) | 1573.6 | 1574.8 | 1576.6 | 1568(15) |
| 83 | 1881.50(7) | 1881.54(10) | 1880.8 | | 1886.3 | 1876(14) |
| 92 | 2245.92(9) | 2246.0 | | | 2255.1 | |

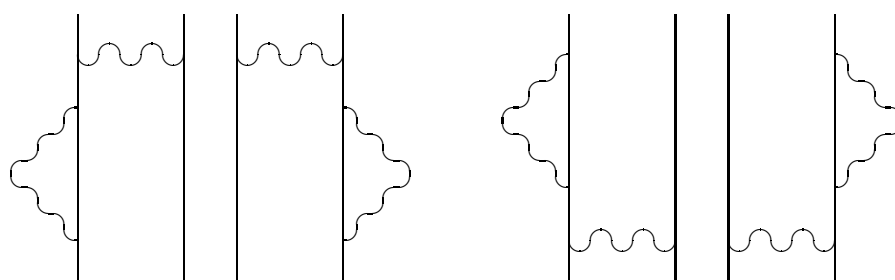
taken from [1].

^a

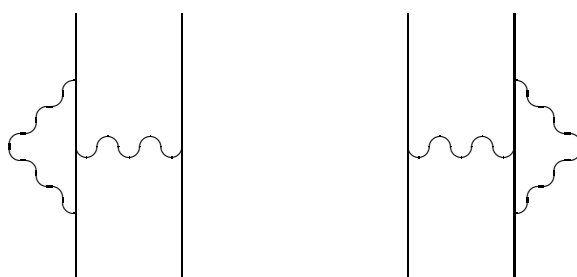
Table 4: Theoretical contributions to the ground state energy of $^{238}\text{U}^{90+}$, without higher order one-electron QED corrections.

| Contribution | Value [eV] | Uncertainty [eV] |
|------------------------|------------|------------------|
| One-electron Dirac | -264559.97 | ± 0.08 |
| One-electron nuc. size | 397.62 | ± 0.76 |
| One-electron nuc. rec. | 1.02 | ± 0.10 |
| One-electron nuc. pol. | -0.40 | ± 0.10 |
| 1st order self-energy | 710.09 | |
| 1st order vac. pol. | -177.20 | |
| 1-ph. exchange | 2265.88 | ± 0.01 |
| 2-ph. exchange non-QED | -12.09 | |
| 2-ph. exchange QED | -0.79 | |
| Self-energy screening | -9.78 | |
| Vac. pol. screening | 2.63 | |
| ≥ 3 -ph. non-QED | 0.06 | |
| ≥ 3 -ph QED | 0.00 | ± 0.09 |
| Two-electron nuc. rec. | -0.01 | ± 0.01 |
| Total | -261382.9 | ± 0.8 |

Figure 1: Two-electron self-energy diagrams.



a



b